Symmetry Protected Topological Semimetals

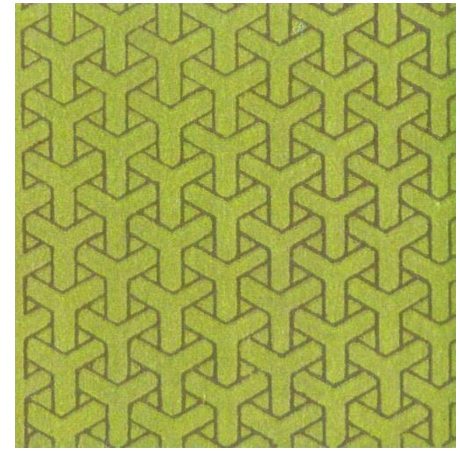
Charles Kane, University of Pennsylvania

Organizing Principles for Understanding Matter

Symmetry

- What operations leave a system invariant?
- Distinguish phases of matter by pattern of broken symmetries

symmetry group p4



symmetry group p31m

Topology

- What stays the same when a system is deformed?
- Distinguish topological phases of matter

genus = 0

genus = 1

Interplay between symmetry and topology has led to new understanding of quantum electronic phases of matter.

Symmetries and Interactions in Topological Matter

Many examples of topological band phenomena

Topological insulators
Chern insulators
Weak topological insulators
Topological crystalline insulators
Topological (Dirac and Weyl) semimetals …..

Many real materials and experiments

Beyond Band Theory: Strongly correlated states

Topologically ordered states
- fractional quantum numbers
- topological degeneracy, quantum information

Symmetry protected topological states

Surface topological order

Much recent conceptual progress, but theory is still far from the real electrons

Topological Superconductivity

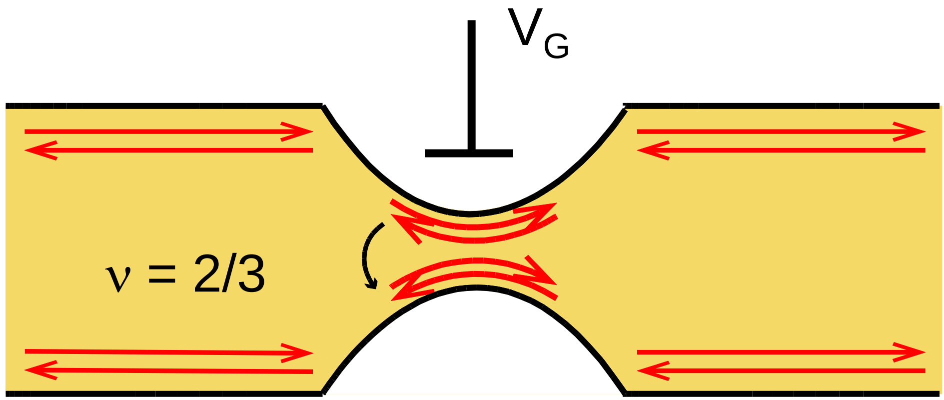
Proximity induced topological superconductivity

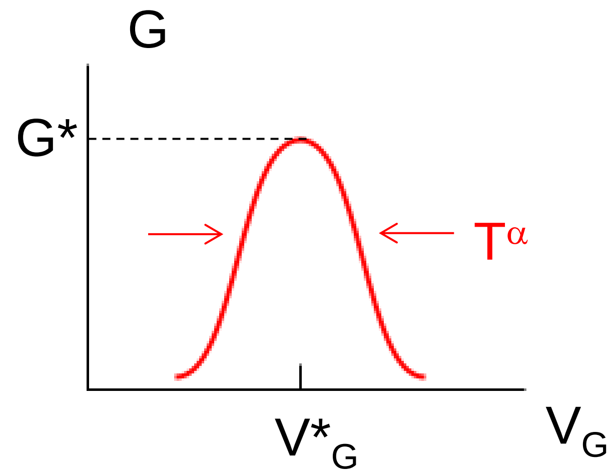
Majorana bound states, quantum information

Tantalizing recent experimental progress

Advertisement: Poster: Yichen Hu

Resonant Tunneling in a Luttinger Liquid





Perfect Resonance = Strongly Interacting
Symmetry Protected
Topological Quantum Critical Point

ν=2/3 FQHE
g_ρ=1/3, g_σ=1 LL

SU(3)$_2$ Kondo fixed point (~ SU(2)$_3$)

Symmetry Protected Topological Semimetals

I. Introduction

II. Dirac Semimetal in 3 and 2 dimensions

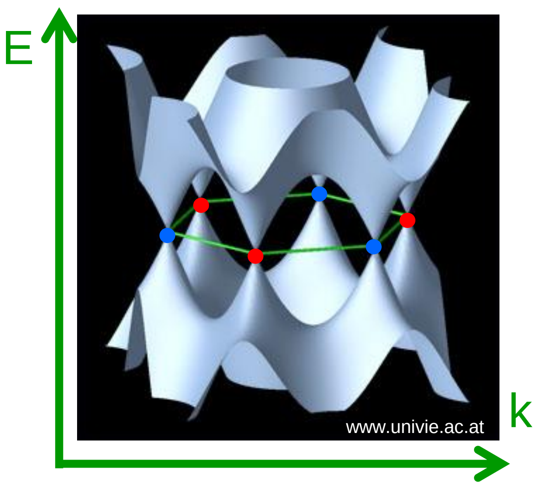
with Andrew Rappe
Gene Mele — U Penn.
Saad Zaheer
Steve Young — NRL

II. Dirac Line Node Semimetal

with Andrew Rappe
Youngkuk Kim — U Penn.
Ben Wieder

Graphene

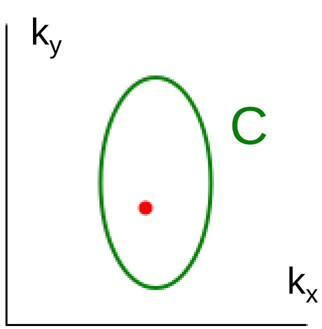
Prototype Symmetry Protected Topological Semimetal



Dirac points protected by

- Inversion symmetry (P)
- Time reversal symmetry (T)
- Absence of spin-orbit (T^2=+1)

Z_2 topological invariant



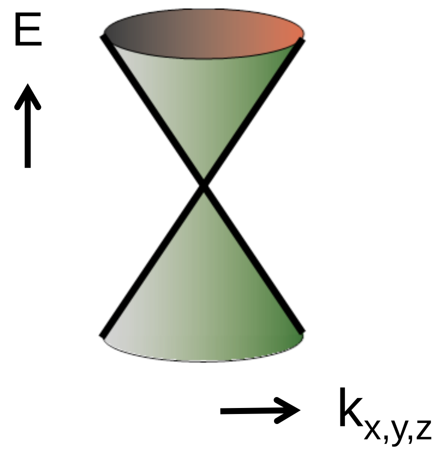
Berry Phase : $\gamma_C = 0 \text{ or } \pi$

3D Weyl/Dirac Semimetals

Weyl semimetal $H = \mathrm{v}\vec{\sigma}\cdot\mathbf{k}$

Wan, Turner, Vishwanath, Savrasov PRB '11
Burkhov, Balents, PRL '11

- 2 fold point degeneracy
- topologically protected, but
  "symmetry prevented" (e.g. break T or P)



Dirac semimetal $H = \mathrm{v}\vec{\gamma}\cdot\mathbf{k}$

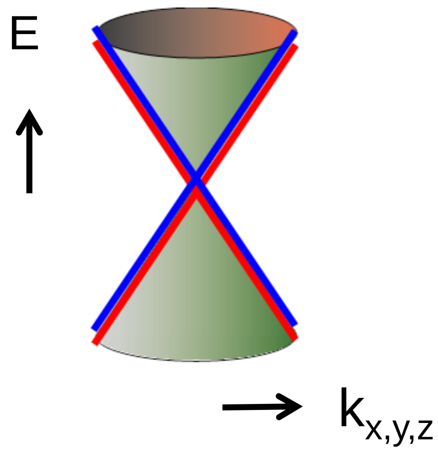
- 4 fold "symmetry protected" point degeneracy
  protected by T, P and other spatial symmetries
- Two distinct classes with different properties

I. Symmetry Point "non-symmorphic" Dirac Semimetals

Young, Zaheer, Teo, Kane, Mele, Rappe, PRL '12

II. Symmetry Line "topological" Dirac Semimetals

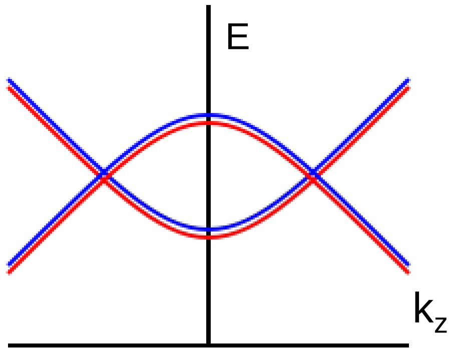
Wang, Sun, Chen, Franchini, Xu, Weng, PRB '12



“Topological” Dirac Semimetal

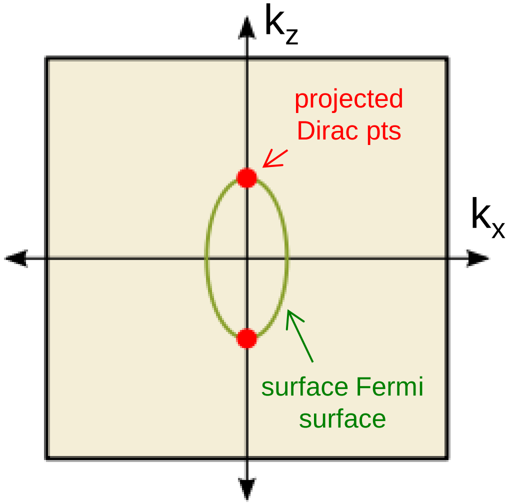
Dirac Points on a line via band inversion

- Consequence of band inversion in presence of spin orbit and C_3 rotational symmetry
- Located on C_3 rotation invariant line in Brillouin zone due to band inversion of opposite parity states in presence of spin orbit and C_3 rotational symmetry



Almost a topological insulator

- Opening a gap by lowering symmetry leads to TI
- Surface states similar to topological insulator



Realizations

- Predicted and observed in Na_3Bi and Cd_2As_3

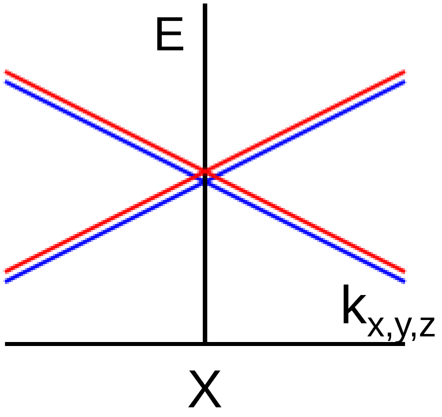
Wang, Sun, Chen, Franchini, Xu, Weng, PRB ‘12
Wang, Weng, Wu, Dai, and Fang, PRB ‘13

Liu, Zhou, Zhang,Wang, Weng, Prabhakaran, Mo, Shen, Fang, Dai, Science ‘14
Liu, Jiang, Zhou, Wang, Zhang, Weng, Prabhakaran, Mo,Peng, Dudin, Nat Mater ’14
Borisenko, Gibson, Evtushinsky, Zabolotnyy, Buchner, Cava, PRL 14

“Non-Symmorphic” Dirac Semimetal

Symmetry Protected Dirac Point

- Located at T invariant point on Brillouin zone boundary
- Protected (and guaranteed) by non-symmorphic symmetry
- Symmetry tuned to transition between topological and trivial insulator : Lowering symmetry (e.g. by strain) can lead to either TI or I



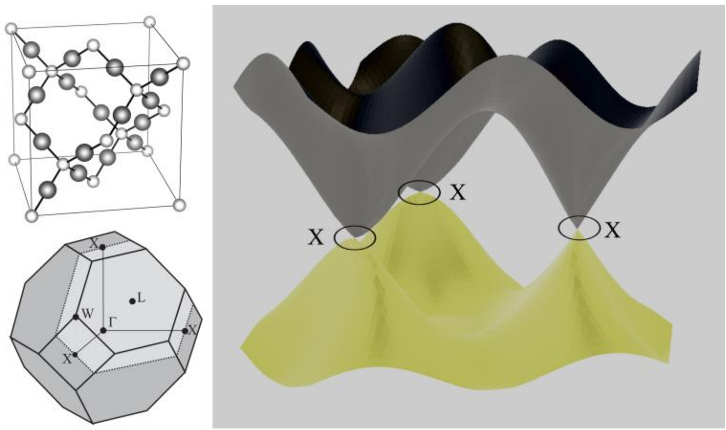
Realizations:

- Toy model: diamond lattice

  Fu, Kane, Mele, PRL ‘07

- Predicted (not yet observed) in BiO_2, $BiZnSiO_4$

  Young, Zaheer, Teo, Kane, Mele, Rappe PRL ’12
  Steinberg, Young, Zaheer, Kane, Mele, Rappe PRL ‘14



BiO_2

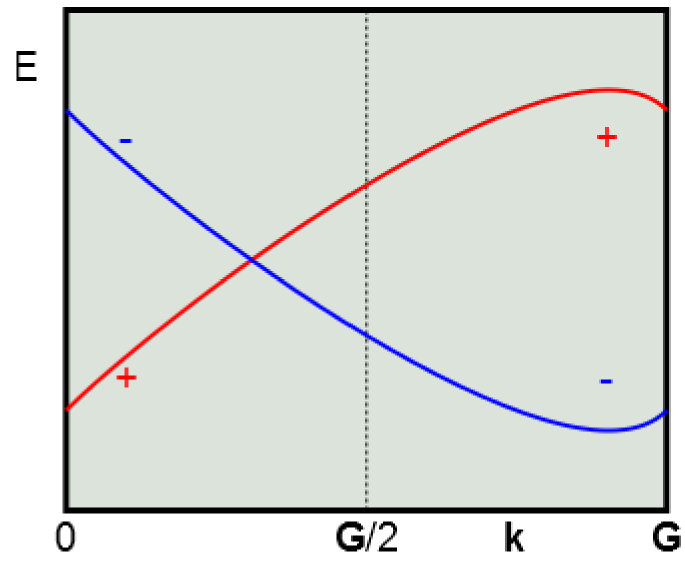
Non-Symmorphic Symmetry

Simplest examples: Glide Plane, Screw Axis

- {g|**t**} :   point group operation g + fractional translation **t**
- On g invariant line (plane), $\{g\,|\,\mathbf{t}\}\left|u_{\mathbf{k}}^{\pm}\right\rangle = \pm\lambda e^{i\mathbf{k}\cdot\mathbf{t}}$, with $e^{i\mathbf{G}\cdot\mathbf{t}} = -1$
- Guarantees bands “stick together”

No additional symmetries :

- Two bands cross between **k** and **k**+**G**



Non Symmorphic Symmetries

Glide Plane, Screw Axis:

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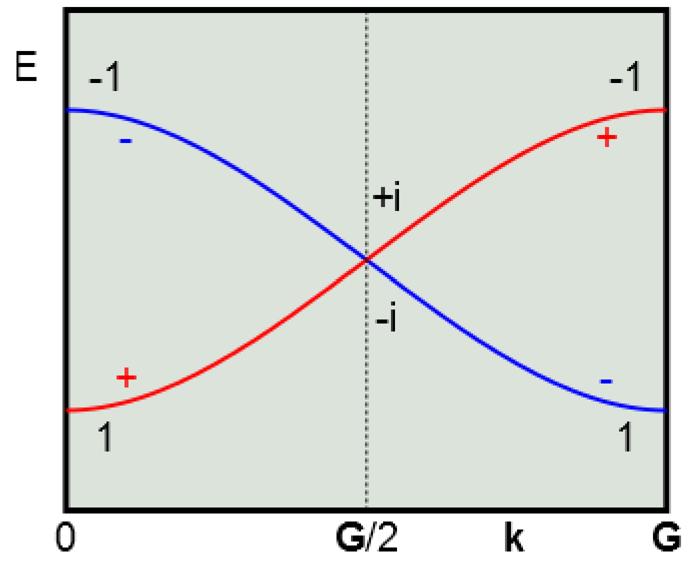
Time reversal (T^2=+1):

- Crossing at zone boundary **G**/2



Non Symmorphic Symmetries

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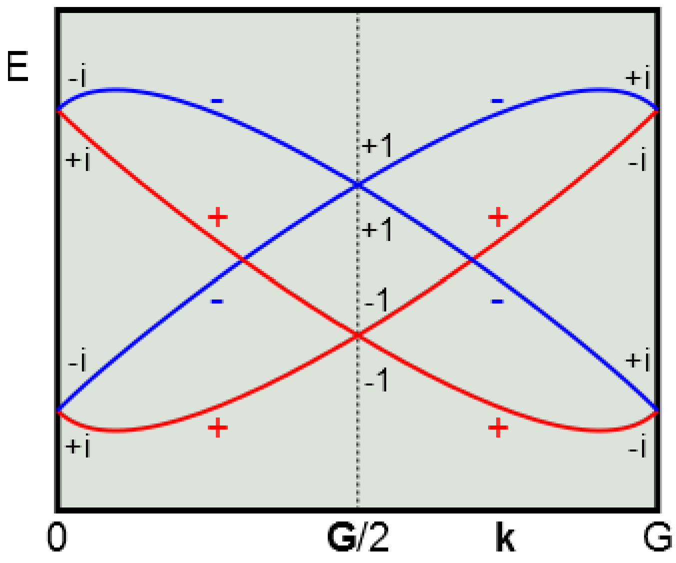
Time reversal (T^2=+1):

- Crossing at zone boundary **G**/2

Time reversal (T^2=-1):

- Kramers degeneracies split by spin-orbit
- Four bands cross between **k** and **k**+**G**



Non Symmorphic Symmetries

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Time reversal (T^2=-1):

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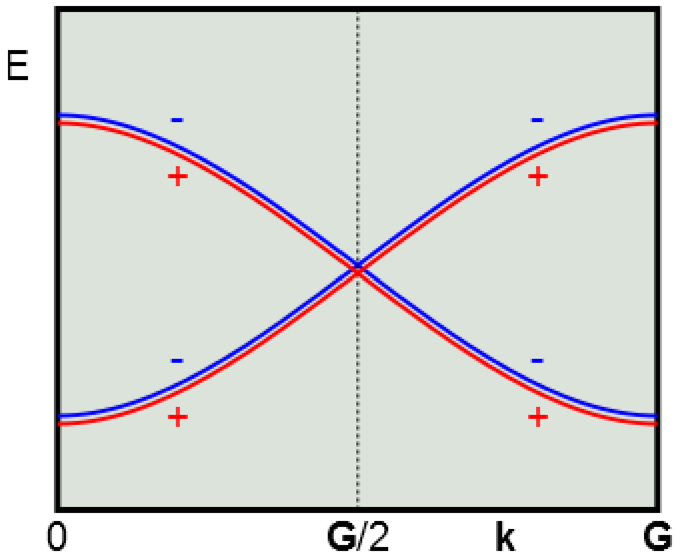
- Four bands cross between **k** and **k**+**G**

Inversion P and T (T^2=-1):

- Degenerate crossing at zone boundary **G**/2

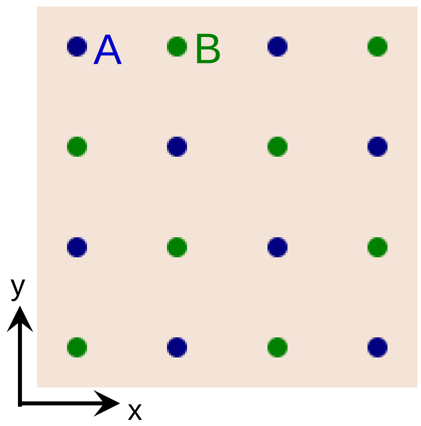


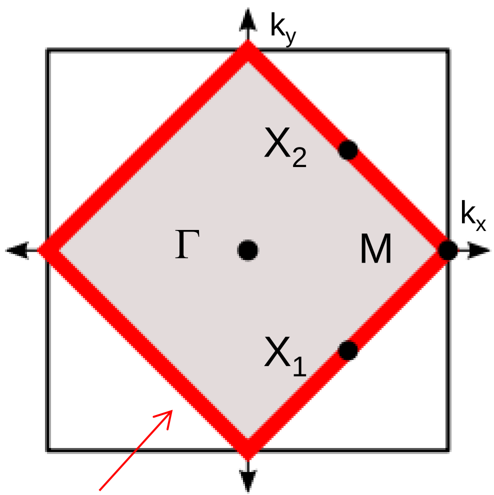
2D Dirac Semimetal

SM Young and CL Kane, arXiv:1504.07977

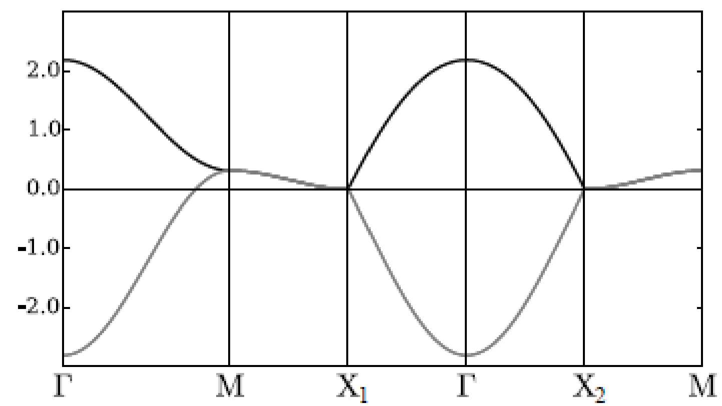
- 2D Dirac points with strong spin orbit interaction
- Symmetry tuned to transition between 2D Topological and Trivial Insulator
- Toy model :   Deformed Square lattice

Undeformed square lattice (doubled unit cell)





Fermi surface



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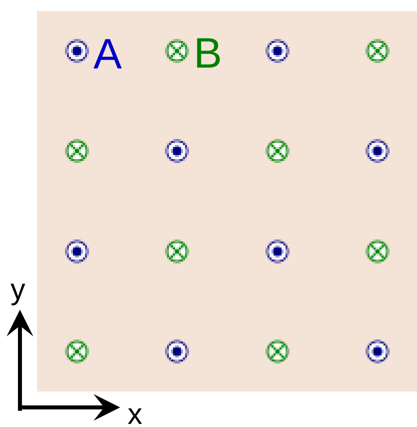
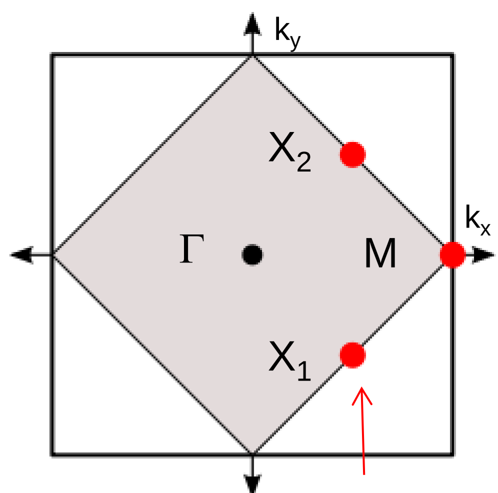
- Toy model : Deformed Square lattice

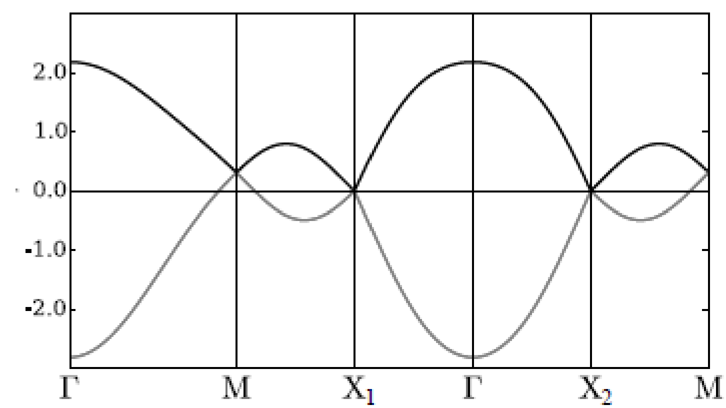
Out of plane deformation: allows 2nd neighbor spin-orbit $i\lambda_{so}\vec{\sigma}\cdot(\mathbf{d}_1\times\mathbf{d}_2)$

Non-symmorphic screw symmetries





3 Dirac Points
Symmetry Inequivalent



2D Dirac Semimetal

SM Young and CL Kane, arXiv:1504.07977

- 2D Dirac points with strong spin orbit interaction
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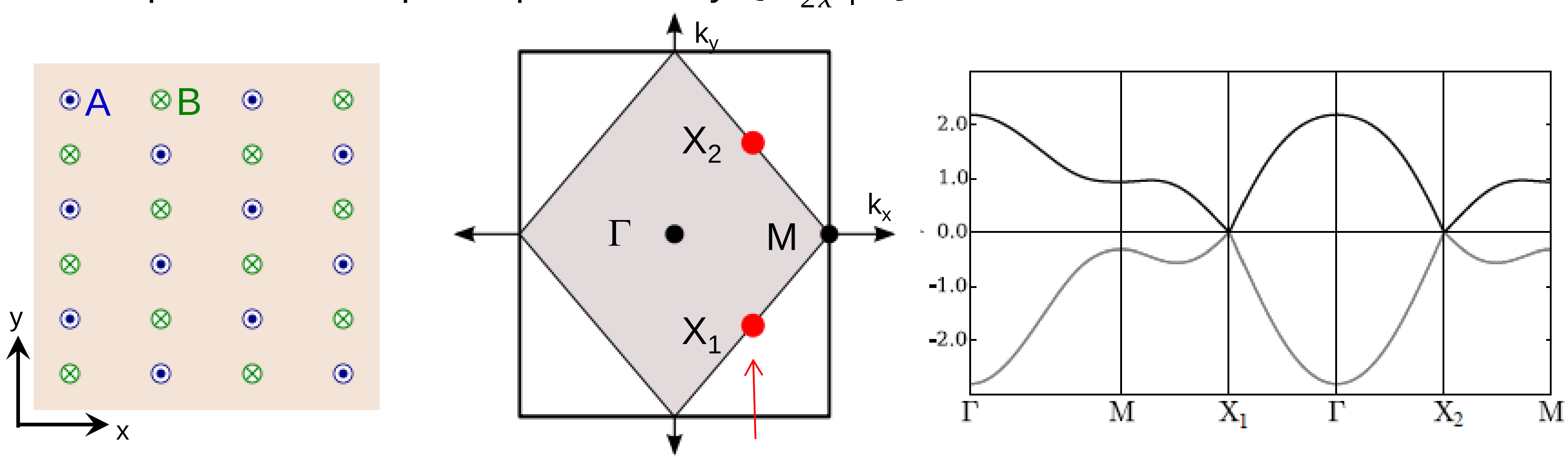
- Toy model :   Deformed Square lattice

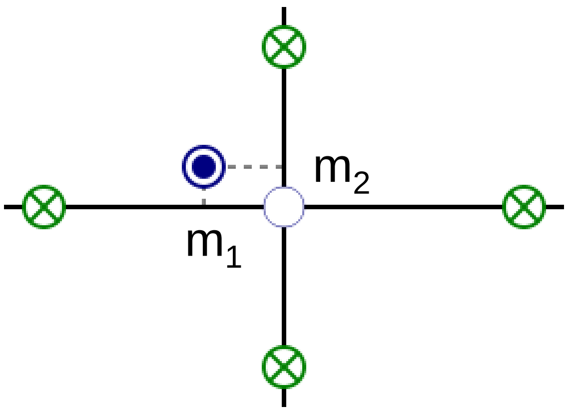
Lower symmetry further:

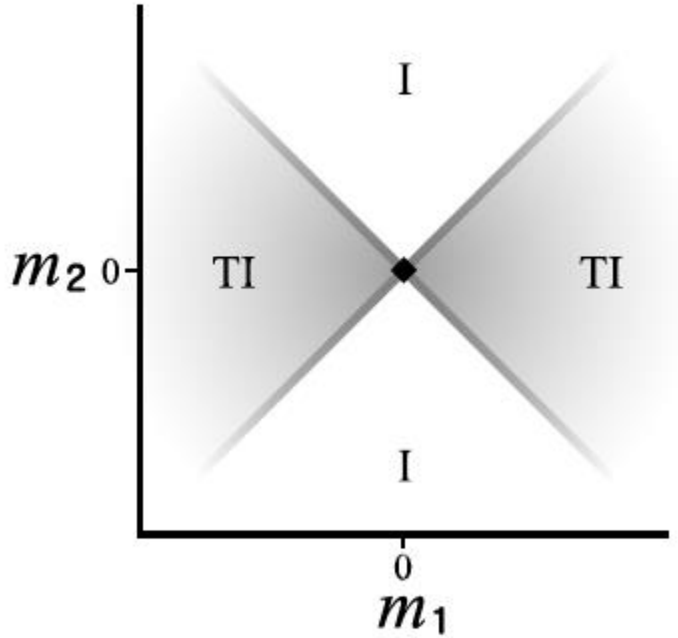
Two equivalent Dirac points protected by $\{C_{2x} \mid \hat{x}\}$



2 Dirac Points
Symmetry Equivalent

Symmetry Tuned Critical Point





- $m_1 \pm m_2$ determine gaps at two Dirac points.
- TI and I are not symmetry related.
- Single symmetry protected Dirac point not possible (except on surface of weak topological insulator or topological crystalline insulator).

Possible Realization

PHYSICAL REVIEW B **90**, 195145 (2014)

Topological phases in iridium oxide superlattices: Quantized anomalous charge or valley Hall insulators

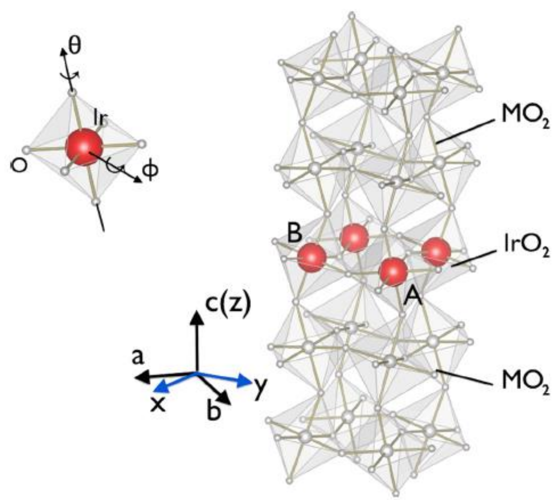
Yige Chen[1] and Hae-Young Kee[1,2,*]

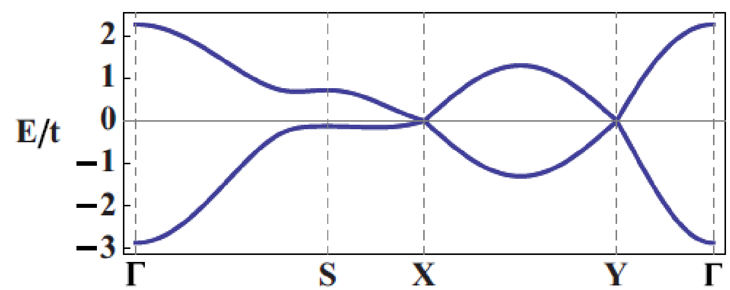
[1] *Department of Physics, University of Toronto, Ontario, Canada M5S 1A7*

[2] *Canadian Institute for Advanced Research, CIFAR Program in Quantum Materials, Toronto, Ontario, Canada M5G 1Z8*

(Received 23 June 2014; revised manuscript received 4 October 2014; published 24 November 2014)

Iridium oxide superlattice grown along [001] with certain rotations of IrO_6 octahedra.

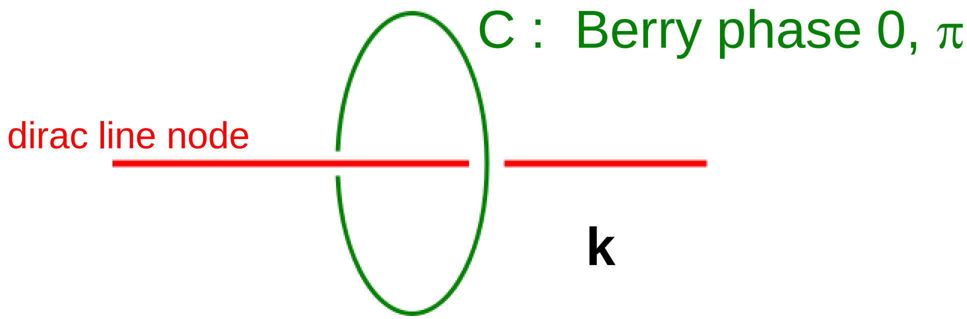




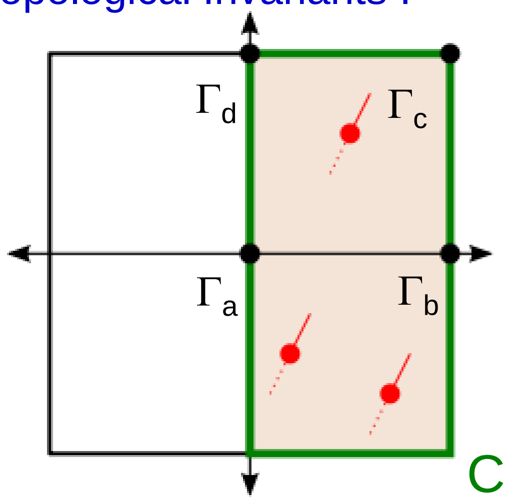
(b) Finite ϕ with b-glide symmetry

3D Dirac Line Node Semimetal

In absence of spin-orbit, P and T ($T^2 = +1$) allows symmetry protected line nodes.



Z$_2$ Topological Invariants :



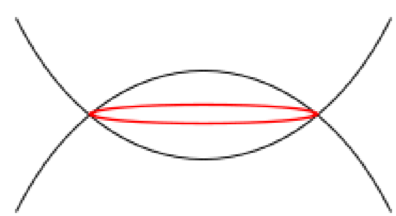
N_{abcd} = # DLN passing through P,T invariant plane spanned by $\Gamma_{a,b,c,d}$

$$(-1)^{N_{abcd}} = \xi_a \xi_b \xi_c \xi_d \qquad \xi_a = \prod_n \xi_n(\Gamma_a)$$ parity eigenvalues

Similar to invariants for TI and WTI with spin orbit

Band Inversion:

Inversion of opposite parity bands leads to a Dirac Circle

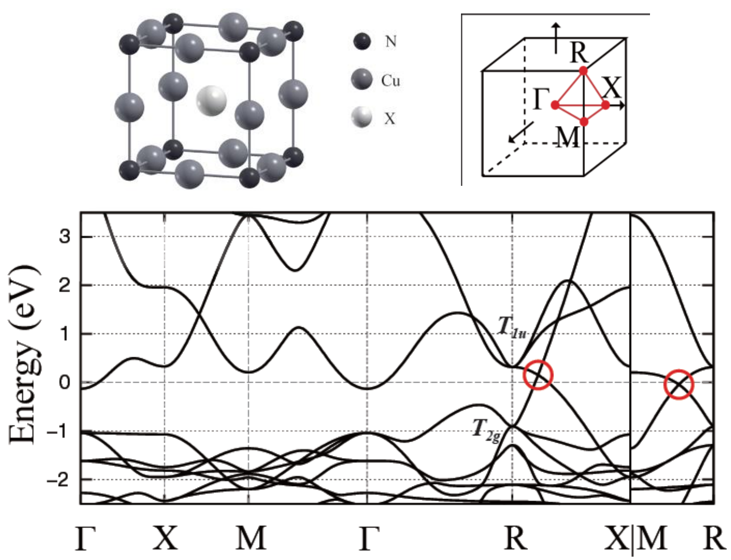


Realizations

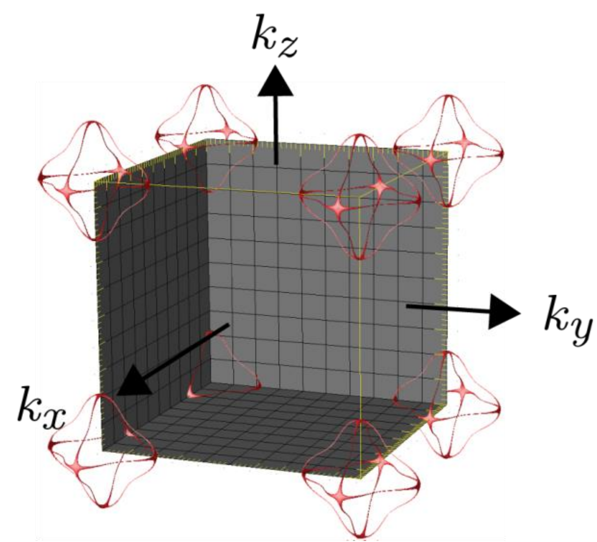
Ca_3P_2 Xie, Schoop, Seibel, Gibson, Xi, Cava, arXiv: 1504.0173 (2015)

Cu_3N Kim, Wieder, Kane, Rappe, arXiv: 1504.03807 (2015)
Yu, Weng, Fang, Dai, Hu, arXiv:1504.04577 (2015)

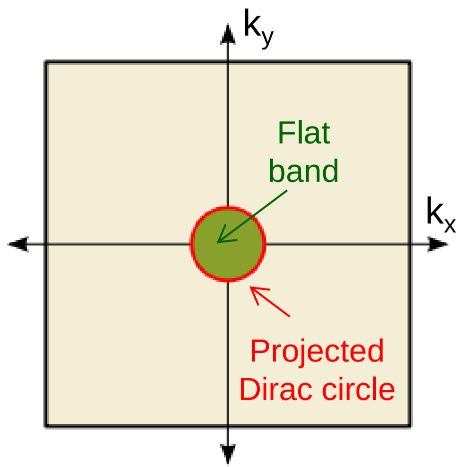
Cu_3N : Uninverted insulator
Band inversion can be controlled by doping with transition metal atoms X



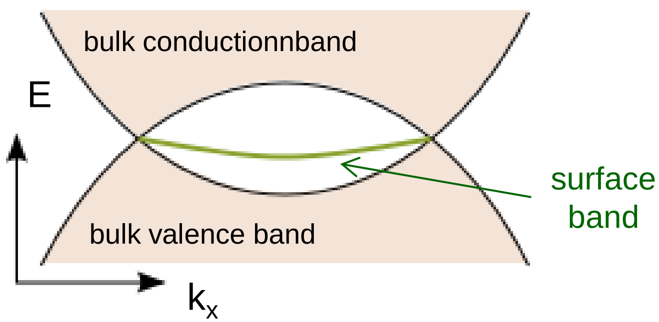
Cu_3N Pd



Nearly Flat Surface Bands



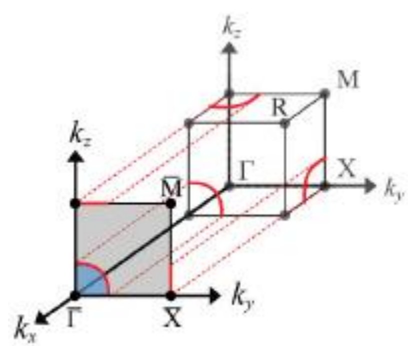
Surface Brillouin Zone

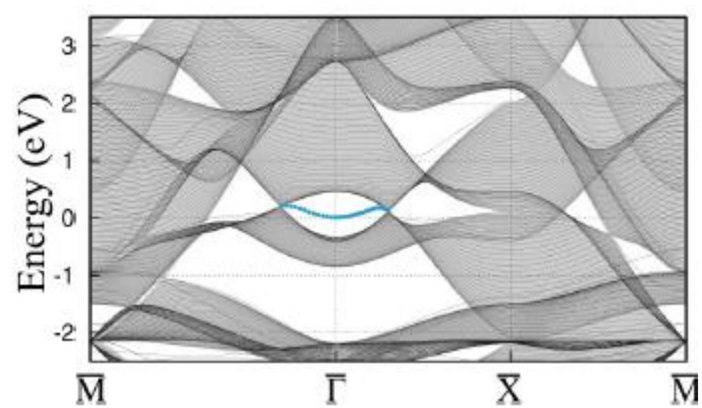


- Curvature of surface band depends on effective masses: $\frac{1}{m_{surf.}} = \frac{1}{m_c} - \frac{1}{m_v}$
- Surface is electrically neutral when surface band is half filled.
- Interesting platform for strong correlation physics.

Cu_3N Zn

slab calculation :





Conclusion

Dirac Semimetals come in two varieties

- “topological” Dirac semimetals
- “non-symmorphic” Dirac semimetals

2D Dirac Semimetal

- Protected by non-symmorphic symmetry
- At intersection between topological and trivial insulator

3D Dirac line node semimetal

- Driven by band inversion in absence of spin-orbit
- Dirac Circle
- Nearly flat surface bands